

LDOS modulations in cuprate superconductors with competing AF order: the temperature effect

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Based upon a phenomenological $t - t' - U - V$ model and using Bogoliubov-de Gennes equations, we found that near the optimal doping $\delta = 0.15$ at low temperature (T), only the pure d -wave superconductivity (dSC) prevails and the antiferromagnetic (AF) order is completely suppressed. However, at higher T the AF order with stripe modulation and the accompanying charge density wave (CDW) emerge, and they could exist even above the superconducting transition temperature. This implies that the existence of the CDW depends critically on the presence of the AF order, not so much on the dSC. The LDOS (local density of states) image indicates that the stripe modulation has an energy independent spacing of $5a/4a$ spreading over a $24a \times 48a$ lattice, corresponding to an average periodicity $4.8a$. This result may be relevant to the recent STM experiment [Vershinin *et al.*, Science **303**, 1995 (2004)].

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Recently, STM measurement by Vershinin *et al.* [1] on slightly underdoped BSCCO indicated that the electronic states at low energies and at a temperature T higher than the superconducting transition temperature (T_c) in the pseudogap region exhibit an energy-independent spatial modulation which resulting to a checkerboard pattern with incommensurate periodicity $4.7a \pm 0.2$ (a is the lattice constant). At very low temperature, however, no such pattern has been detected [1], in agreement with previous measurements [2, 3]. So far the reasons why this STM pattern at low temperature looks so different from that at high temperature, and why the noninteger incommensurate periodicity could occurred in a under-line CuO_2 lattice are outstanding questions which have not been addressed in the existing literatures. In the present paper we are trying to understand these issues by adopting the idea of the d -wave superconductivity (dSC) with a competing antiferromagnetic (AF) order for cuprate superconductors [4, 5, 6, 7, 8, 9], and to examine the formation of the AF order and the accompanying charge density wave (CDW) at finite temperature. Employing the phenomenological $t - t' - U - V$ model with proper chosen parameters, we show that at low temperature only dSC prevails in our system and the AF order is completely suppressed. The LDOS (local density of states) image is featureless. At higher temperature, it is found that the AF order with stripe modulation, which is referred also as the spin density wave (SDW), and the accompanying charge density wave (CDW) may show up and they could even persist at temperatures above the BCS superconducting transition temperature T_c^{BCS} . In the presence of SDW, we show the LDOS image to have an energy-independent stripe modulation with spacing of $5a/4a$ spreading over a $24a \times 48a$ lattice. According to the Fourier analysis of the LDOS image, an average periodicity $4.8a$ could be assigned for the stripe modulation. If the doubly degenerate states of x - and y -

oriented stripes have the same probability to appear in the time interval when the experiments is performed, the combined LDOS image should have a checkerboard pattern of $4.8a \times 4.8a$ structure. This result is in agreement with the experiment by Vershinin *et al.* [1]. In addition, the temperature dependent behavior of the normalized LDOS, exhibits the "pseudogap"-like characteristics [10] originated in the emergence of the SDW at higher T .

To model these observed phenomena, we employ an effective mean-field $t - t' - U - V$ Hamiltonian by assuming that the on-site repulsion U is responsible for the competing antiferromagnetism and the nearest-neighbor attraction V causes the d -wave superconducting pairing

$$\begin{aligned} \mathbf{H} = & - \sum_{\mathbf{ij}\sigma} t_{\mathbf{ij}} c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + \sum_{\mathbf{i}\sigma} (U \langle n_{\mathbf{i}\bar{\sigma}} \rangle - \mu) c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{i}\sigma} \\ & + \sum_{\mathbf{ij}} (\Delta_{\mathbf{ij}} c_{\mathbf{i}\uparrow}^\dagger c_{\mathbf{j}\downarrow}^\dagger + \Delta_{\mathbf{ij}}^* c_{\mathbf{j}\downarrow} c_{\mathbf{i}\uparrow}), \end{aligned} \quad (1)$$

where $t_{\mathbf{ij}}$ is the hopping integral, μ is the chemical potential, and $\Delta_{\mathbf{ij}} = \frac{V}{2} \langle c_{\mathbf{i}\uparrow} c_{\mathbf{j}\downarrow} - c_{\mathbf{i}\downarrow} c_{\mathbf{j}\uparrow} \rangle$ is the spin-singlet d -wave bond order parameter. The Hamiltonian above shall be diagonalized by using Bogoliubov-de Gennes' (BdG) equations,

$$\sum_{\mathbf{j}}^N \begin{pmatrix} \mathcal{H}_{\mathbf{ij}\sigma} & \Delta_{\mathbf{ij}} \\ \Delta_{\mathbf{ij}}^* & -\mathcal{H}_{\mathbf{ij}\bar{\sigma}}^* \end{pmatrix} \begin{pmatrix} u_{\mathbf{j}\sigma}^n \\ v_{\mathbf{j}\bar{\sigma}}^n \end{pmatrix} = E_n \begin{pmatrix} u_{\mathbf{i}\sigma}^n \\ v_{\mathbf{i}\bar{\sigma}}^n \end{pmatrix}, \quad (2)$$

where $\mathcal{H}_{\mathbf{ij}\sigma} = -t_{\mathbf{ij}} + (U \langle n_{\mathbf{i}\sigma} \rangle - \mu) \delta_{\mathbf{ij}}$. Here, we choose the nearest-neighbor hopping $\langle t_{\mathbf{ij}} \rangle = t = 1$ and the next-nearest-neighbor hopping $\langle t_{\mathbf{ij}} \rangle = t' = -0.25$ to match the curvature of the Fermi surface for most cuprate superconductors [12]. The exact diagonalization method to self-consistently solve BdG equations with the periodic boundary conditions is employed to get the N positive eigenvalues (E_n) with eigenvectors ($u_{\mathbf{i}\uparrow}^n, v_{\mathbf{i}\downarrow}^n$) and N negative eigenvalues (\bar{E}_n) with eigenvectors ($-v_{\mathbf{i}\uparrow}^{n*}, u_{\mathbf{i}\downarrow}^{n*}$). The

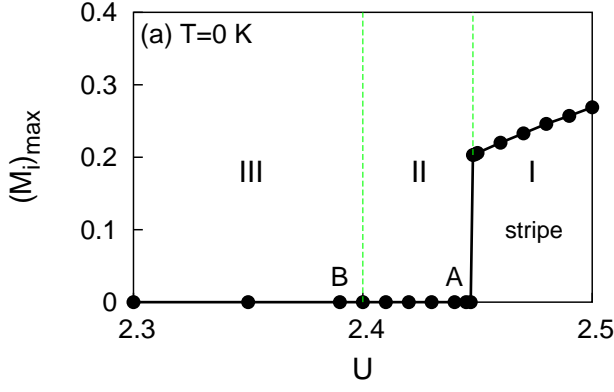


FIG. 1: The maximum value of the staggered magnetization $(M_i)_{max}$ as a function of U at zero temperature, where $M_i = (-1)^i(n_{i\uparrow} - n_{i\downarrow})$. The size of the unit cell is $N_x \times N_y = 48 \times 24$.

self-consistent conditions are

$$\begin{aligned} \langle n_{i\uparrow} \rangle &= \sum_{n=1}^{2N} |\mathbf{u}_i^n|^2 f(E_n), \quad \langle n_{i\downarrow} \rangle = \sum_{n=1}^{2N} |\mathbf{v}_i^n|^2 [1 - f(E_n)], \\ \Delta_{ij} &= \sum_{n=1}^{2N} \frac{V}{4} (\mathbf{u}_i^n \mathbf{v}_j^{n*} + \mathbf{v}_i^{n*} \mathbf{u}_j^n) \tanh\left(\frac{\beta E_n}{2}\right), \end{aligned} \quad (3)$$

where $\mathbf{u}_i^n = (-v_{i\uparrow}^{n*}, u_{i\uparrow}^n)$ and $\mathbf{v}_i^n = (u_{i\downarrow}^{n*}, v_{i\downarrow}^n)$ are the row vectors, and $f(E) = 1/(e^{\beta E} + 1)$ is Fermi-Dirac distribution function. Since the calculation is performed near the optimally doped regime, the filling factor, $n_f = \sum_{i\sigma} \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle / N_x N_y$, is fixed at 0.85, i.e., the hole doping $\delta = 0.15$. Each time when the on-site repulsion U or the temperature μ needs to be adjusted.

In Fig. 1, we plot the maximum value of the staggered magnetization $(M_i)_{max}$ as a function of U with $V = 1.0$ at $T = 0$. The value of U measure the strength of the competing AF order in the background of the dSC. In region I, where $U > U_c \sim 2.45$, the AF order with stripe modulation or the SDW shows up and it has a period $8a$ oriented along the x - or y -axis. The corresponding modulations in dSC and accompanying CDW have a period $4a$. All these have been discussed in one of our earlier works [13]. In regions II and III, where $U < U_c$, the AF order is completely suppressed by the dSC and $(M_i)_{max} = 0$, and the system is in the pure dSC state. The transition between the stripe-modulated dSC/SDW/CDW coexisting state and the pure dSC state is discontinuous and of the first order. The difference between region II and region III is that in the presence of an applied magnetic field, dSC/SDW/CDW with stripe modulations are induced in region II while in region III two dimensional modulations are induced around the vortex cores. Detailed study of this issue has been given previously [14] and will not be discussed here. In the following, we choose $U = 2.44$ (region II) which is slightly smaller than the critical U_c and $U = 2.39$ (region III) to examine their temperature

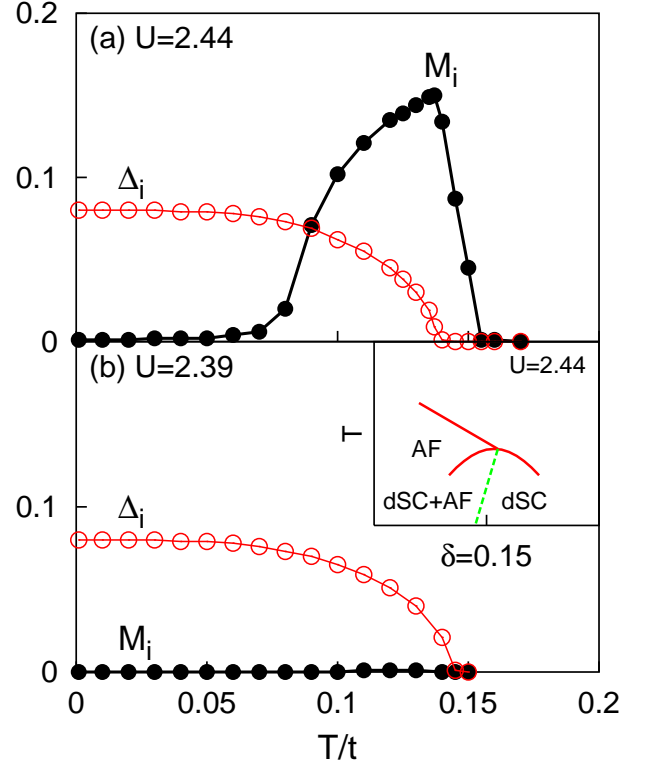


FIG. 2: (a) and (b) show the temperature dependence of the dSC (open circle) and AF order (solid circle), respectively, for $U = 2.44$ and $U = 2.39$. The value of the dSC order parameter $\Delta_i = \frac{1}{4}(\Delta_{i+\hat{x}} + \Delta_{i-\hat{x}} - \Delta_{i+\hat{y}} - \Delta_{i-\hat{y}})$ is measured in the unit of t and $M_i = (M_i)_{max}$.

effects.

Fig. 2 shows the temperature dependences of the dSC order (open circle) and the staggered magnetization $(M_i)_{max}$ (solid circle) for (a) $U = 2.44$ and (b) $U = 2.39$. From Fig. 2(a), it is straightforward to see that only dSC exists and the AF order is completely suppressed at low T . When $T > 0.06t$, the stripe-modulated AF order and the accompanying CDW start to emerge, and both of them could persist above the BCS transition temperature $T_c^{BCS} = 0.14t$. This result implies that the existence of the CDW depends critically on the presence of the AF order, not so much on the dSC. At $T > T_c^{BCS}$, the staggered magnetization decreases rapidly to zero at the Néel's temperature $T_N = 0.155t$. We also found that the stripe modulation associated with the SDW has mixed periods $10a/8a$, and those associated with the dSC and the accompanying CDW have a mixed periods $5a/4a$ oriented either along the x -axis or the y -axis. Within the temperature range in which the AF order appears, these periods seem to be temperature insensitive. In Fig. 2(b), with $U = 2.39$, the AF order is completely suppressed and our system is in the state of pure dSC at all temperatures. In both of these cases, the dSC order parameter as a function of T appears to have the BCS-like behavior. It is interesting to note that the T_c^{BCS} in the case

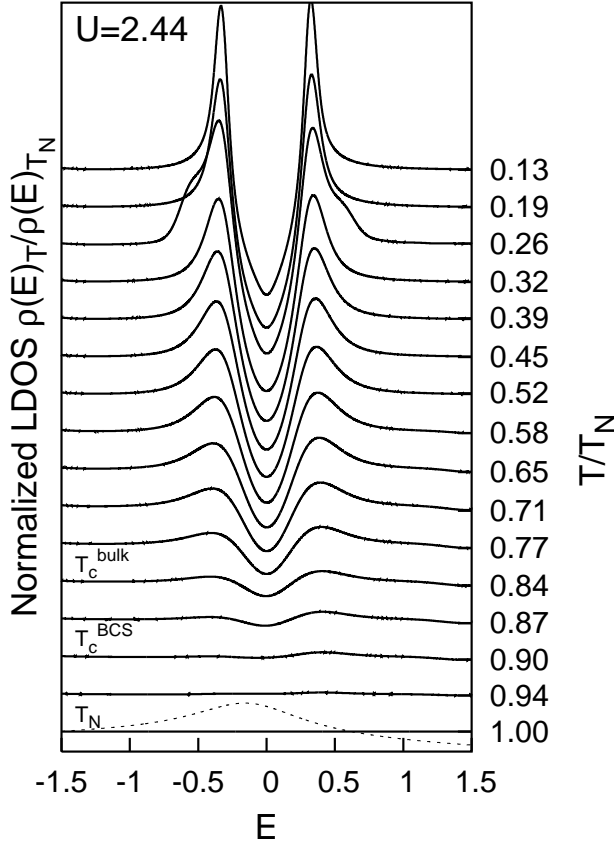


FIG. 3: Temperature dependence of the normalized LDOS ($\rho_i(E)_T/\rho_i(E)_{T_N}$, here $T_N = 0.155t$). The LDOS at T_N as a function of E is represented by the dashed line. This representative set of spectra was shifted vertically for clarity. The wavevectors in first Brillouin Zone are $M_x \times M_y = 24 \times 12$.

for $U = 2.39$ [Fig. 2(b)] is slightly larger than the one for $U = 2.44$ [Fig. 2(a)]. This is because the appearance of SDW in Fig. 2(a) at higher T also suppresses the dSC. The reason why the AF order is suppressed at low temperature and emerges at higher temperature could be understood from the phase diagram for $U = 2.44$ near the optimal doping which is shown in the inset of Fig. 2(b). The feature of this phase diagram is similar to what has been obtained for dSC with competing d -density wave (dDW) order [15].

The LDOS is defined as

$$\rho_i(E)_T = -\frac{1}{M_x M_y} \sum_{n,\mathbf{k}} \left[\left| \mathbf{u}_i^{n,\mathbf{k}} \right|^2 f'(E_{n,\mathbf{k}} - E) + \left| \mathbf{v}_i^{n,\mathbf{k}} \right|^2 f'(E_{n,\mathbf{k}} + E) \right], \quad (4)$$

where $\rho_i(E)_T$ is proportional to the local differential tunneling conductance as measured by STM experiment, and the summation is averaged over $M_x \times M_y$ wavevectors in first Brillouin Zone. In order to investigate the continuous evolution of the quasiparticle spectrum, the LDOS

for $U = 2.44$ from low T to high T are calculated. The normalized LDOS which is defined as $\rho_i(E)_T/\rho_i(E)_{T_N}$, are presented in Fig. 3 as a function of energy E and at temperatures ranging from $T/T_N = 0.13$ up to $T/T_N = 1.0$. It should be noticed that $T_c^{bulk} (< T_c^{BCS})$ labeled in Fig. 3 corresponds to the temperature where the coherent peaks of the dSC flatten out, and this signature has been used to estimate the "superconductivity transition temperature" in many experiments. As it is indicated in Fig. 3 that the apparent "gap" is roughly a constant up to T_c^{bulk} and progressively becomes slight larger up to T_N , in consistent with the experimental measurements [16]. As far as the temperature behavior of the normalized LDOS is concerned, the essential feature of Fig. 3 displays the "pseudogap"-like characteristics. In the temperature range of $T_c^{bulk} < T < T_N$, our system appears to be in the "pseudogap" region according to the characterization from STM experiments [10, 11] even though the effect due to the phase fluctuations on the dSC order parameter [17, 18] has not been taken into account. In this region, the Fermi surface in our theory is everywhere gaped while the ARPES experiment [19] indicates that the gaps occur only near $(\pm\pi, 0)$ and $(0, \pm\pi)$. This difficulty so far has not been solved in the existing literatures.

In order to compare with the STM experiment, we calculate the LDOS images between the energy 0.0 and 0.4 with the increment 0.01. At the temperature $T/T_N = 0.94$, which is larger than T_c^{BCS} and in the "pseudogap" region, we found that the LDOS images have stripe modulations with mixed periods of $5a/4a$ which is energy independent. The periods of stripes spread into $5a - 5a - 4a - 5a - 5a$ pattern oriented along either the x -axis or the y -axis on a 24×48 lattice. The system seems trying to establish a periodicity that is incommensurate with the underline lattice, but fails to do so because the calculation is performed in a discrete and finite lattice, not in a continuum. In Fig. 4(a), we show such an image at $E = 0.1$. The pattern in Fig. 4(a) still remains even as the temperature drops to $T = 0.08t$ [Fig. 2(a)]. As it will be shown below that an average periodicity $4.8a$ for the stripe modulation could be assigned in this case. The x - and y -oriented stripe modulations are degenerate in energy and it is thus possible to use the minima of a double-well potential to represent the states of the x - and y -oriented stripes. Since the modulations discussed here are weak perturbations to the host system, we do not expect that the barrier in the mid of the double-well potential to be large and the tunneling between these two degenerate states could be achieved easily by quantum mechanics and thermal activation. When both x - and y -oriented stripe-modulations show up in the time duration when the experiment is performed, checkerboard patterns should be observed.

In order to get a further understanding of stripe modulation, let us investigate the Fourier transform of the

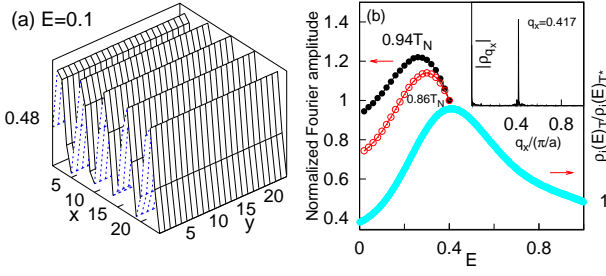


FIG. 4: (a) The LDOS image at $E = 0.1$ and $T = 0.94T_N$. (b) The energy evolutions of the Fourier amplitude at $T = 0.94T_N$ (solid circle) and $T = 0.86T_N$ (open circle) of the LDOS image at $q_x = 0.417(\frac{\pi}{a})$, and the LDOS at $T = 0.94T_N$. The insert in (b) is the Fourier amplitude of the LDOS image in (a). The wavevectors which have been used to calculate the LDOS image are $M_x \times M_y = 12 \times 12$ in first Brillouin Zone.

LDOS image

$$\rho_{\mathbf{q}}(E)_T = \frac{1}{\sqrt{N_x N_y}} \sum_{\mathbf{i}} \exp(i \mathbf{q} \cdot \mathbf{r}_{\mathbf{i}}) \cdot \rho_{\mathbf{i}}(E)_T. \quad (5)$$

The Fourier transform of the LDOS image in Fig. 4(a) as a function q_x is displayed in the insert of Fig. 4(b). It shows a very sharp peak around $q_x = 0.417(\frac{\pi}{a}) = \frac{2\pi}{4.8a}$, corresponding to an average "periodicity" $4.8a$ in real space. At $T = 0.94T_N > T_c^{BCS}$ and in Fig. 4 (b), the curve represents the LDOS of a function of energy while the solid/open circle shows the energy evolution of the Fourier amplitude of the LDOS image at $q_x = 0.417(\frac{\pi}{a})$, which are normalized by their values at $E = 0.4$. Starting from the higher energy side, the solid circle first rises to a maximum at $E = 0.27$ and then dips as E approaches to zero. This energy dependence is predicted for the case where we only have SDW/CDW without dSC in presence. When the temperature is lowered to $T = 0.86T_N < T_c^{BCS}$ where dSC/SDW/CDW are all in coexistence, a result represented by the open circle is obtained for the Fourier amplitude of the LDOS image. If one introduces an additional parameter to consider the effect of phase fluctuations on the dSC order parameter, the dip in the low energy side of the open circle might be removed and flattened after reaching the maximum [20] and the obtained result could agree better with the STM measurement [1]. A simplified procedure of doing this has been previously proposed [18] and we are not going to repeat this again in the present paper. It also necessary to mention here that a different work has also been done by Chen *et al.* [20] for rather underdoped sample ($\delta = 0.125$) to address a similar issue. Their periodicity $4a$ in the LDOS modulation shows up at all temperatures below the BCS transition temperature.

In conclusion, we have investigated the interplay between the dSC and the competing AF/CDW orders at finite temperature for samples close to the $\delta = 0.15$ doping. With proper chosen parameters, we show that the

AF order could be completely suppressed by the dSC at low T , and the LDOS image is featureless. At higher T , the AF and the accompanying CDW orders start to emerge and they persists even to temperatures higher than T_c^{BCS} . This finding implies that the presence of CDW depends on the existence of AF order, not so much on the dSC. When the AF order emerges, stripe like modulations appear in all AF/dSC/CDW orders and also in the LDOS image. It is shown that the normalized LDOS from low T to high T exhibits the "pseudogap"-like behavior. The Fourier transform of the LDOS image is peaked around $\mathbf{q} = (2\pi/4.8a, 0)$ indicating a periodicity $\sim 4.8a$ for y -oriented stripes. Moreover the energy independent checkerboard pattern which was observed by Vershinin *et al.* [1] at high T but not at low T could be understood in terms of the present theory if both the x - and y -oriented stripes contribute in the time interval when the experiment is performed. Finally we point out that for a different sample which may have a U slightly larger than 2.44 (see Fig. 1 in region I) or a hole-doping level slightly less than 0.15, stripe modulations with period $4a$ would show up at $T = 0$. This result should be consistent with the energy-independent checkerboard patterns observed in other STM experiments [21].

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